

THE CENTER FOR MOLECULAR MODELING AND COMPUTATIONAL QUANTUM CHEMISTRY – CMMCQC

Code of Conduct for the Computing Resources

1. User profile

The CMMCQC clusters are the computing resources for The Center for Molecular Modeling and Computational Quantum Chemistry, a small user community interested in research in computational chemistry, physics, biology and engineering in Cluj-Napoca, located at the Chemistry Department of the Babes-Bolyai University (BBU) and administered jointly with staff from the Cluj-Napoca Technical University (CNTU). It is not:

- * a general facility.
- * a general BBU or CNTU facility.
- * a general resource for all chemistry applications.
- * a replacement for your own computer.

CMMCQC users are expected to be experienced computational chemists/engineers/biologists/physicists who aim to push back the frontiers of the field. They should know how to use a computer efficiently and they should have their own computing facilities to back the computing power of the CMMCQC. In particular, they should be adequately equipped to do the (interactive) pre- and postprocessing of calculations and have sufficient peripheral resources (disk space, visualization, printer, plotter, graphics, text processing...) to carry out their research.

Users are expected to protect their account by non-trivial passwords (e.g., such that cannot be deduced from the data known about account owner and that is not a name of a person, animal or object). If the password is revealed or lost, it is necessary to change it ASAP and to inform a system administrator. Strange behavior of your account, appearance or disappearance of files, unknown processes running under your identity must be reported to the administrators.

2. Policy

We aim to make work as simple as possible for the users. In particular, we want to avoid the implementation of strict restrictions (disk space, cpu time, etc.) and cumbersome administrative procedures. This, however, will only work if users are willing to cooperate. Hence, these guidelines.

Accounts for the different CMMCQC machines are personal. However, an account owner may let another CMMCQC user who is a member of his/her research group make use of his/her account occasionally or for a limited period of time. Nevertheless, the account owner and the research group leader are held responsible for all actions originating in the account. Trespassing of the CMMCQC rules can be met with closing the account.

Where required for acknowledgements in scientific publications, the users are hereby informed that the CMMCQC resources have been supported by the Romanian Government via the CAPACITATI project No. 130/14.09.07 (2007-2009).

3. Application Software

Normally, no support for application software should be expected from the system administrators. General-purpose computational software for chemistry will usually be found installed and working on CMMCQC computers. If you need to install a special software package, contact CMMCQC administrators. However, depending on the nature of your request, you may have to be prepared to order, pay for, and possibly install and maintain your favorite package yourself. In order to avoid duplication, check with system administrators for packages already available (<http://chem.ubbcluj.ro/pagini/anorganica/isi/capacitati/index.html>).

4. Assistance

The system administrators cannot offer any assistance or advice beyond fixing technical problems. Novices have to be looked after by more experienced users in their group. Courses and support on Linux and programming languages are offered by BBU, and system administrators will direct you in this respect.

5. Running jobs

In order to provide maximum throughput and turnaround for all users, jobs have to be run in batch queues. Job queues reflect the requirements of classes of applications and the capabilities of the workstation configurations. Do inform yourself on the configuration of the queuing systems on the CMMCQC clusters via the general information pages of the clusters (<http://chem.ubbcluj.ro/pagini/anorganica/isi/capacitati/index.html>).

Rules:

- * Keep the number of your jobs in the queues within reasonable limits.
- * Stick to the queue appropriate for your job.
- * No interactive/background jobs!

6. Disk space

There are several categories of disk space:

- * User home directories are on the file server, there are quota, home directories are backed up.
- * Temporary space on the file server with a life time of several days, no backup.
- * Scratch space on the compute servers is short-time space, which has to be cleaned up as soon as possible by the user. It is not safe, not included in the backup, and will be wiped without notice if space is needed. If necessary, scratch space is wiped after every job.

Rules:

- * Please note that there is no large long-time disk space on the CMMCQC clusters. Store those data on your home machine.
- * Clean up after yourself. Scratch space is the fastest space and it is precious. Keep it available to the jobs after yours. Temporary space on the file server is intended to keep data between two jobs, not as long-term storage.
- * If you keep your home directory small, you will help us very much.

* Cooperate with above policy. We would like to avoid draconic measures like quota on temporary space, automatic deletion of files and so on. To that end, we need your goodwill and cooperation.

7. Human relations

The CMMCQC user community is small. You probably know most of the other users. If you are unhappy with another user, please contact them directly before you complain to the system administrators.

8. Closing of accounts

In order to keep accounting and system administration as lean as possible, and in order to avoid uncontrolled accounts (for security reasons), CMMCQC users leaving their current research groups are kindly asked to inform one of the system administrators. Accounts that have not been used for 9 months will be closed by the system administrator without further notification. After an additional wait time of 3 months, data belonging to these accounts will be deleted.

9. Whom to contact? Addresses and Responsibilities

The CMMCQC has three leaders, who oversee the scientific usage of the CMMCQC, identify funding sources for system maintenance and upgrades, and take decisions on these issues based on the advice of the System Administrators. Decisions on the structure and usage rules of the computing resources will require a consensus of the three project leaders. It is the responsibility of the project leaders to oversee the observation of the present Rules of Conduct, and the responsibility of the system administrators to enforce them on a day-to-day basis.

CMMCQC project leaders:

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